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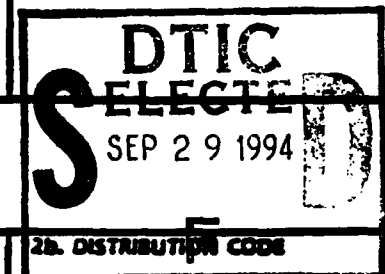
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We have investigated the interactions of hyperthermal (few to several hundred eV) atomic ions with metal surfaces, in particular the dynamics of electron transfer between the particle and surface. Progress is reported in the following areas: 1) construction of a time-of-flight spectrometer for measuring energy- and angle-resolved distributions of neutral and charged alkali atoms. 2) measurements of the magnitude and velocity-dependence of the neutralization probabilities for Li, Na, and K scattered from clean Cu(001); dramatic differences for Li, Na, and K reflect the sensitivity of nonadiabatic charge transfer to the energies and lifetimes of atomic electronic states near the surface. 3) measurements of branching ratios for Li^+ , Li^- and ground- and excited-state ($\text{Li}(2s)$ & $\text{Li}(2p)$) formation in Li^+ scattering from alkali-covered Cu(001), which provide a test of new multi-state charge transfer models and indicate some of the first evidence of multi-state effects in atom-surface charge transfer. 4) extensions of our multi-state studies to include formation of higher energy excited states of Li and Na, and multiple states in O^+ and O_2^+ scattering. 5) observation of trajectory-dependent charge transfer for 50 eV Na^+ scattering from clean Cu(001); evidence is found for modification of the neutralization due to collision-induced defect formation in the surface. 6) preliminary measurements of trapping probabilities for 10-100 eV Na^+ scattering from clean Cu(001), which show a strong nonmonotonic dependence on the incident energy. These studies are part of a new program to investigate the mechanisms by which hyperthermal energy ion beams can be used to modify thin film growth.

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RESONANT CHARGE TRANSFER IN HYPERTHERMAL ATOMIC
AND MOLECULAR ION-SURFACE COLLISIONS

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I. SUMMARY

Section I of this report gives a comprehensive summary of our research program to investigate the interactions of hyperthermal energy (a few eV to several hundred eV) and low energy (keV) ions with clean and adsorbate-covered surfaces. We have investigated fundamental collision and charge transfer dynamics; these are important for understanding processes which occur in a wide variety of applications involving ion-surface collisions at hyperthermal energies. For example, for understanding surface reactions in the space environment (e.g., shuttles in low earth orbit), scattering, and trapping dynamics at incident energies of 10 eV and lower are of particular interest. Hyperthermal energy ions of a few hundred eV and lower are also widely used in surface processing techniques such as reactive ion etching, ion beam-assisted and direct ion beam thin film deposition, and surface modifications by plasma processing and deposition.

In the studies described below, a particular emphasis was placed on *ion-surface charge exchange processes*. Charge exchange, the transfer of electrons between the scattering atom and the surface, is an essential step in many gas-surface dynamical processes, such as energy transfer, trapping, adsorption, and molecular dissociative chemisorption. It plays a key role in some examples of laser-induced desorption and laser-induced surface reactions. Charge transfer is also of direct importance in sputtering processes, and poisoning and promotion of chemical reactions. Our goal was to obtain experimental *information about charge transfer mechanisms*. The experiments are accompanied by theoretical calculations which enable us to probe detailed dynamics of charge transfer processes. We can extract information about fundamental nonadiabatic electronic interactions of atoms (or molecules) and surfaces: e.g., how atomic levels shift and broaden due to interactions with the surface electronic states, and the role of the particle velocity and surface work function in determining how charge is transferred between the atom and surface.

In more recent and continuing experiments, we are extending our studies to specifically address the role of energy and charge transfer processes in ion-assisted and direct ion beam deposition of thin films. It is well documented that the use of hyperthermal ions in thin film growth can lower growth temperatures, change growth kinetics, and alter the morphology, structure and properties of the deposited film; fundamental collision processes that modify thin film growth include energy transfer, trapping, embedding, and charge transfer. Future studies will be directed toward understanding these growth modifications.

Comprehensive Summary of Results

We have obtained results in the following areas, some of which were covered in our interim reports submitted in February 1992, March 1993, and April 1994, and others that will be covered in detail below. Relevant references to published results are given.

1. Development of a neutral and ion alkali detector

We developed and tested a time-of-flight spectrometer for energy- and angle-resolved detection of neutral and charged low and hyperthermal energy alkalis. Neutral detection at hyperthermal energies is a difficult experimental problem; we developed a quantitative detection scheme in which the neutral alkalis are ionized by scattering from a high work function surface, after which they can be easily detected using standard channel electron multiplier techniques [1,2]. Using biasing elements to reject charged particles, we can separately determine ion and neutral fractions. This enables us to measure absolute yields of neutrals and ions in the scattered flux. This detector was crucial in our studies of charge transfer processes. At sufficiently high energies, the detector can also be used for quantitative detection of neutral fractions of other species as well, such as oxygen. The detector and its operation were covered in detail in the 1992 and 1993 reports and in references [2,3].

2. Velocity-dependent neutralization of Li, Na, and K scattering from clean Cu(001)

Neutralization probabilities were measured for Li, Na, and K scattering from clean Cu(001) over a range of final particle velocities; i.e., for a given final angle and velocity we measured the probability with which the different alkali species would leave the surface as an ion or as a neutral [3]. The incident beam energies ranged from 5 eV to 1600 eV. The magnitudes of the neutralization probabilities, and how they vary with final velocity of the scattered particle, were very different for Li, Na, and K. These data were compared to calculated neutralization probabilities derived from a "one-electron" model of the resonant charge transfer process; good qualitative agreement with the data was obtained. This model, developed by Brako and Newns, describes the relatively simple case where transfer occurs primarily to one electronic level in the scattered particle.

This work demonstrates that the neutralization probabilities are very sensitive to the energies and widths of atomic resonances near the surface. The experiments also provide important experimental tests of charge transfer models, and theoretical calculations of atomic state widths and energies [4-6]. We have also demonstrated that the neutralization probability for 5-1200 eV Na scattering from Cu(001) is sensitive to the component of the scattered particle's velocity that is parallel to the surface. This behavior was initially unexpected and can be understood using a modified version of the one-electron model discussed above; the motion of the atom with respect to the surface changes the charge transfer probabilities because, from the rest frame of the atom, the energies of the metal electrons are doppler shifted. These studies were covered in the 1992 and 1993 reports and references [3,7,8].

3. Multi-state effects in charge transfer for Li^+ scattering from Cs and K covered Cu(001)

In item 2 above we found good qualitative agreement with measured neutralization probabilities for Li, Na, and K scattering from clean Cu(001) using a model which treated the interaction of one atomic state (the ionization level) with the surface. Modeling that treats a single atomic state, however, is an approximation since charge transfer involves the simultaneous interaction of several atomic states with the surface electronic states. To understand these multi-state interactions in more detail, we have made measurements of branching ratios to different final electronic states for Li^+ scattering from alkali-covered Cu(001) surfaces. In the scattered flux we observed Li^+ , Li^- , $\text{Li}(2s)$ (ground state neutrals), and $\text{Li}(2p)$ (excited state neutrals). With theorist Brad Marston from Brown University, we have analyzed these data using a many-body resonant charge transfer model [8-12] that treats the simultaneous interactions of several atomic states with the surface and includes electron correlation effects. Unlike the one-electron model discussed above, this model can treat the case where multiple final electronic states are formed via charge transfer processes.

Early results from this work were discussed in the 1993 and 1994 reports and references [8-12]. Over the past year we have made considerable progress. Measurements have been made involving the formation of higher energy (than $\text{Li}(2p)$) excited states and the formation of excited states in Na scattering. The data have been analyzed in greater detail, giving better insight into the dynamics of multi-state charge transfer processes. Recent extensions of the model have improved its accuracy and enable us to include Auger charge transfer processes (as well as resonant). These recent results will be summarized in section III.

4. Charge transfer for O_2^+ and O^+ scattering

We have measured charge transfer for scattering of O_2^+ from clean and adsorbate-covered Cu(001), and for scattering of O^+ from clean Cu(001). We have observed the formation of O^- and O_2^- resulting from O_2^+ collisions with clean and adsorbate-covered surfaces. Following calibration of our ion detector, we have made quantitative measurements of the O^-/O^+ yields for O^+ scattering from clean Cu(001). These results were covered in the 1992 and 1993 reports.

We are currently analyzing these yields using models developed by Peter Nordlander and Brad Marston. Planned modifications to the detector described above will enable us to *directly* detect scattered neutral oxygen, which becomes the dominant channel at low energies.

5. Trajectory-dependent charge transfer for 50 eV Na^+ scattering from clean Cu(001)

We have observed "trajectory-dependent" neutralization for Na^+ scattering from clean Cu(001); for 50eV and 7.5eV incident Na energies, we have observed neutralization probabilities that vary from 0.07 to 0.5 for particles that have the same outgoing velocity and angle, but different collisional histories. This was an unexpected result since, at the low particle velocities used in these experiments, one expects that the charge exchange probabilities will be determined by the final particle velocity. To our knowledge, these results

represent the first report of trajectory-dependent neutralization from a clean surface. Modeling indicates that the differences in neutralization are due to the type of collision the particle experienced at the surface. For the 50 eV scattering, the particle penetrates to the second layer, from which it scatters away from the surface, thus leaving the surface through a region in which top layer atoms have undergone significant lateral displacements. On the other hand, for the 7.5 eV scattering the particle scatters from the top layer only and leaves from a relatively unperturbed region of the surface. The surface atom displacement in the 50 eV scattering has associated with it a significant perturbation in the local surface electrostatic potential; it can be thought of approximately as a vacancy in the surface which is electronically screened. Modeling which includes an estimate of this electronic perturbation gives good agreement with the measured results. These results were summarized in the 1994 report and in references [13].

6. Particle trapping and thin film growth modification at hyperthermal energies

It is well documented that the use of hyperthermal ions in thin film growth can lower growth temperatures, change growth kinetics, and alter the morphology, structure, and properties of the deposited films. We have initiated both scattering and scanning tunneling microscopy (STM) studies [14–17] to investigate the *mechanisms by which energetic ions modify growth processes*. Important fundamental ion-surface interactions that will play a role in growth modification include energy transfer, trapping, embedding, and charge transfer. Through the use of classical trajectory simulations and the development of ion-surface interaction potentials, we can describe energy transfer from the ion to the surface in detail: how much energy is deposited and how it is initially partitioned among the surface atoms. In a recent series of experiments we have also studied 10-100 eV sodium trapping on Cu(100). The trapping probability is a strongly nonmonotonic function of the incident energy [18].

Ultimately our goal is to incorporate our understanding of charge transfer into a more complete description of the dynamics of scattering at hyperthermal energies, i.e., to determine the role that charge transfer plays in energy transfer to the surface and particle trapping. Future experiments will address these issues in the context of thin film growth applications. Below we briefly discuss ongoing and planned experiments.

II. RESEARCH OBJECTIVES

Our research objectives under grant number AFOSR-91-0137 were as follows:

1. To develop instrumentation for quantitative measurements of branching ratios to different final electronic states of hyperthermal energy atoms and molecules scattered from clean and adsorbate-covered surfaces.
2. To use these measured branching ratios to probe basic mechanisms of charge transfer for alkalis scattered from clean copper surfaces. Charge transfer calculations are used to extract information about the energies and widths of atomic electronic resonances near surfaces, and to probe the dynamics of multi-channel charge transfer processes.
3. To extend the knowledge we have gained about nonadiabatic charge transfer pro-

cesses for the relatively simple alkali-Cu systems to more complex systems, such as oxygen scattering from metal surfaces. These latter cases require more sophisticated experimental and theoretical treatments.

4. To initiate studies of the role of hyperthermal energy ions in thin film growth modification. Fundamental processes we will study include energy transfer, charge transfer, trapping, and embedding of particles in ion-assisted and direct ion beam deposition of thin films.

III. STATUS OF RESEARCH

Recent results from this research are outlined briefly below and can be found described in more detail elsewhere (relevant references are given).

Charge Transfer Dynamics in Ion-Surface Collisions

Motivation:

Charge transfer, or the exchange of electrons, between an atom or molecule and a surface at small separations can occur by one of a number of processes: e.g., resonant electron tunneling, Auger, or direct radiative transfer. For a particle that scatters, desorbs, or sputters from a surface, charge transfer can result in a change in the particle's charge state and/or the formation of excited states [3]. Such processes give rise, for example, to distributions of final electronic states in SIMS (secondary ion mass spectrometry), and in some laser-induced and electron-induced (ESD) desorption processes. Charge transfer processes are also a fundamental step in a number of more complex surface processes, including dissociative chemisorption, trapping, and surface chemical reactions.

Charge transfer events are very sensitive to the electronic structure of the specific particle and surface in question. As an atom or molecule approaches a surface, its electronic levels, which have well-defined energies far from the surface, become broadened, shifted, and hybridized resonances near the surface. The widths and energies of these resonances are rapidly varying functions of particle-surface separation z . Thus, at different z , a given resonance is degenerate with different states in the substrate. For example, in the case of a metal substrate, the energy shift may mean that the resonance lies predominantly above the Fermi level on some parts of the trajectory, and below it on others, i.e., in such a case there is a "Fermi level crossing." The widths and energies of different resonances, and whether they are degenerate with filled or empty states in the substrate, are factors which lie at the root of many particle-surface dynamical interactions, whether they be scattering, adsorption, desorption, etc. [1,3,19,20]. The resonance energies and widths are difficult to calculate [4-6] and difficult to access directly by most experimental techniques. They can, however, be studied by scattering experiments, such as those presented below.

Scattering experiments at hyperthermal energies provide a unique opportunity to study charge transfer processes. Branching ratios to different final electronic states can be measured as a function of particle velocity, surface work function, incident species, etc. Modeling can then be used to study the dynamics of the charge transfer.

More specifically, when a particle approaches or leaves the surface at non-zero veloc-

ity, at any given instant the system may or may not be in the adiabatic electronic ground state, depending on various time scales in the collisions. In the hyperthermal energy range the time scales of the collisions can be comparable to the time scales of electron transfer (resonance lifetimes) between the particle and surface, making it possible to nonadiabatically populate different final electronic states on the outgoing trajectory. The faster the scattered particle, the closer to the surface (where the lifetimes are shortest) the final electronic state is determined. Thus, the branching ratios to different final electronic states will vary with velocity. It is often assumed [21,22] that the important velocity component is that which is perpendicular to the surface, v_{\perp} , since the particle-surface coupling is assumed to be a function of z . For a given incident species, the branching ratios will also be sensitive to changes in the Fermi energy (i.e., changes in the work function $\Delta\Phi$) of the substrate. For example, lowering the work function will change where the Fermi level crossings occur, and may bring higher energy atomic states into resonance with occupied surface states. This latter type of experiment is discussed below.

Multi-state effects in resonant neutralization for Li and Na scattering from alkali-covered Cu(001)

We have measured branching ratios to different final electronic states for Li^+ scattering from surfaces with different work functions. The substrate was clean Cu(001). Potassium and cesium adsorbates were used to shift the work function from the clean surface value of 4.59 eV, to values as small as approximately 1.4 eV, i.e., a work function shift, $\Delta\Phi$, of approximately 3.2 eV. The branching ratios for scattering into different final electronic states, in particular Li^+ , Li^- , $\text{Li}(2s)$ (neutral ground state), and $\text{Li}(2p)$ (neutral excited state), were measured as a function of the adsorbate-induced work function shift. In the 1993 interim report and in references [8–12], preliminary results were presented. The key results are highlighted here along with recent progress toward modeling these results and extending the measurements.

Experimental results:

Figure 1 is a plot of the measured probabilities with which an impinging 400 eV Li^+ ion scatters from the Cu(001) surface as a positive ion (P^+) or a negative ion (P^-) versus the work function shift induced by the deposition of Cs [8–10]. The 400 eV Li^+ ions impinge at an angle of $\theta_i = 65^\circ$, measured with respect to the surface normal, and along the $\langle 100 \rangle$ azimuth. The detected particles have been scattered into a final angle of $\theta_f = 64^\circ$, also measured with respect to the surface normal. For the clean surface, P^+ is 0.67 ($v_{\perp} = 0.02$ a.u.). As the work function decreases from its clean surface value of $\Phi = 4.59$ eV ($\Delta\Phi = 0.0$ eV) to a value of about 2.6 eV ($\Delta\Phi \approx -2.0$ eV), P^+ decreases, with a corresponding increase in the probability P^0 with which the Li^+ ion will scatter as a neutral atom (ground state or otherwise). In this range of work function values, P^- is less than a few percent. However, as the work function further decreases, P^- begins to increase at the expense of P^0 . For work function values less than about 2.6 eV, P^+ is less than a few percent.

In addition to the overall charge state fractions presented above, we have determined the relative yield of Li^+ ions scattered into the $\text{Li}(2p)$ state by detecting photons corresponding to the $\text{Li}(2p) \rightarrow \text{Li}(2s)$ transition ($\lambda = 673$ nm) [8–11]. A plot of the relative yield

of Li(2p) versus the cesium-induced work function shift $\Delta\Phi$ is shown in figure 2 for 400eV incident Li^+ (open triangles). (The absolute yields of the Li(2p) states are estimated to be less than 1%.) When the surface is clean (i.e., $\Delta\Phi = 0.0$ eV), we observe no photons. However, as the work function decreases, the photon yield increases, reaches a peak value, and then decreases. The distinctive feature of these data is the peak in the yield at a work function shift of about -1.8 eV. Also shown in figure 2 is the photon yield for 100eV incident Li^+ (closed circles), which also shows a peak in the photon yield as a function of decreasing work function. When the energy is decreased from 400 eV to 100 eV, the peak in the Li(2p) yield decreases by about an order of magnitude and appears at lower work function shifts. A similar peak has been observed when 1 keV Li^+ was scattered at grazing angles from Cs/W(110) [23,24]. Note also in the 100 eV data that there is a second upturn in the relative Li(2p) yield at the lowest work functions, i.e., $\Delta\Phi \approx -3.0$ to -3.2 eV.

Modeling:

To model these experiments we require a charge transfer calculation which can treat the simultaneous interactions of several atomic resonances with the surface electronic states. To accurately include excited atomic states and affinity levels required a many body calculation. Brad Marston (at Brown University) has developed such a model that employs a $1/N$ expansion (equivalent to a variational expansion of the many-body wavefunction in particle-hole pairs) to study the dynamics of multi-state charge transfer. This expansion has been employed with success in the Kondo problem, and by Brako and Newns who earlier applied it to the charge transfer problem [25]. Marston has extended their treatment by including level crossings, excited atomic states and affinity levels. Input to the model includes the energies and widths of the atomic resonances outside the surface. These were taken from calculations by Nordlander and Tully; they are shown in figure 3. We have also used widths for the Li($2s^2$) level calculated by Gauyacq and Teillet-Billy [26,27]. Details of the calculations are given elsewhere [9].

Discussion:

In figure 1 the solid curves represent absolute charge state fractions calculated using Marston's multiple-states model. Shown in figure 2 are the calculated Li(2p) yields. The two curves in figure 2 are for 400 eV (solid line) and 100eV (dashed line) Li scattering. Both calculated curves in figure 2 have been normalized to the data.

The model reproduces the measured absolute yields of positive and negative ions, and qualitatively reproduces the measured peak in the Li(2p) yield, the decrease in the Li(2p) yield as the ion energy is decreased from 400 eV to 100 eV, and the shift in the peak that occurs when the beam energy decreases from 400 eV to 100 eV. Note that the calculated peaks in figure 2 are narrower than the experimental ones; we believe that this is a result of alkali adsorbate-induced inhomogeneities in the surface electrostatic potential, which are not included in the calculation.

Given the agreement between the measured and calculated yields, we can now use the model to extract information about the dynamics of the charge transfer process. A detailed analysis is quite lengthy and is discussed elsewhere [references 8-12]. Key results are summarized below.

Charge state yields, Li^+ and Li^- :

The charge state yields, i.e., yields of Li^+ and Li^- (see figure 1), can be understood by considering the relative energies of the Fermi level and the $\text{Li}(2s)$ (ionization) and $\text{Li}(2s^2)$ (affinity) levels (see figure 3). The Fermi level of clean $\text{Cu}(001)$ lies 4.59 eV below the vacuum level. For a Li atom far from the surface, the $\text{Li}(2s)$ level lies 5.4 eV below the vacuum level, while the $\text{Li}(2s^2)$ lies 0.62 eV below the vacuum. A Li atom which scattered adiabatically from the clean surface would always scatter as a neutral. However, due to the finite velocity of the scattered particles, the final charge states are determined close to the surface (on the order of a few to several angstroms) where the energy of the $\text{Li}(2s)$ level lies above the Fermi level of the clean surface (see figure 3). Thus, a significant Li^+ yield is observed in the scattered flux. As the work function decreases (by adsorbing Cs onto the Cu surface), the Fermi level crossing for the $\text{Li}(2s)$ level moves closer to the surface, and more neutralization occurs. This trend continues until essentially no Li^+ is observed in the scattered flux. Decreasing the work function increases the fraction of the $\text{Li}(2s^2)$ resonance that lies below the Fermi level, which increases the Li^- yield.

Excited state yields, $\text{Li}(2p)$:

The $\text{Li}(2p)$ (see figure 2), in particular the existence of the peak versus $\Delta\Phi$, is a manifestation of multi-state effects in the charge transfer. Since the $\text{Li}(2p)$ level lies 3.54 eV below the vacuum, from energetic considerations, it is not expected to form in Li scattering from clean $\text{Cu}(001)$. As the work function decreases and the Fermi level shifts up in energy, the $\text{Li}(2p)$ resonance becomes degenerate in energy with filled surface electronic states on parts of its trajectory. When this occurs, one expects to see $\text{Li}(2p)$ in the scattered flux. One would naively expect the $\text{Li}(2p)$ yield to increase with decreasing work function. However, both the experiment and calculations give a peak in the $\text{Li}(2p)$ yield, which as we will see below, is a multi-state effect.

Modeling - ground state $\text{Li}(2p)$ occupancy near the surface:

Recall that close to the surface, the atomic and surface electronic states are strongly interacting, i.e., the atomic widths are large. This has several consequences. First, if we were to fix the atom close to the surface, say at $z = 1\text{\AA}$, we would find that the adiabatic ground state of the atom is a hybridized state with admixtures of the metal states, and the $\text{Li}(2s)$, $\text{Li}(2p)$, and $\text{Li}(2s^2)$ (and other) atomic states. Second, since the atomic level widths are so broad, electron transfer times are very short and we expect that close to the surface, even in a scattering experiment, the system reaches electronic equilibrium, i.e., is in the electronic adiabatic ground state [12]. Due to the hybridization that occurs close to the surface, the ground state will have partial occupancies in the different atomic states. We can calculate, for the ground state, the probability that the Li atom is positively or negatively ionized, or is in the 2s or 2p state. These probabilities will depend on the energies of the atomic states relative to the Fermi level, and their widths. As the work function decreases with increasing adsorbate coverage, these probabilities will change. Figure 4 shows the probabilities for finding the atom in different states calculated as a function of $\Delta\Phi$ for a fixed atom-surface separation of 1\AA .

For the clean surface, when the system is in the adiabatic ground state, the Li is predominantly a positive ion P^+ (see figure 4, $\Delta\Phi = 0$), with some admixture of the

Li(2s) ground state neutral $P^{\circ}(2s)$ and the Li(2p) excited state neutral $P^{\circ}(2p)$. For the lowest work functions used in the experiment, i.e., $\Phi = 1.4$ eV, or $\Delta\Phi = -3.2$ eV, the ground state is predominantly a negative ion, P^{-} , with some admixture of the Li(2s) state. These trends are qualitatively what one would expect from simple energetic considerations (see figure 3).

Now focus on the probability for finding the atom in the excited Li(2p) state, $P^{\circ}(2p)$, and how it varies with $\Delta\Phi$. There is some probability of finding the atom in the Li(2p) state on the clean surface, which increases slightly with decreasing work function up to $\Delta\Phi \approx -2.0$ eV. At the lowest work functions, however, the probability for the Li(2p) state decreases, and becomes zero for $\Delta\Phi = 3.2$ eV. Note that the decrease in $P^{\circ}(2p)$ coincides with an increase in the probability of finding the Li^{-} state; i.e., there is a competition with the negative ion state at the lowest work functions which decreases the occupancy of the Li(2p) state close to the surface.

The partial occupancies shown in figure 4 are similar to those that occur in a scattering experiment at the distance of closest approach since, close to the surface where the level widths are broad, electronic equilibrium will be established. Then, on the outgoing trajectory, the occupancies in the different states will evolve as the level widths and energies change (see figure 3). The first conclusion that we can draw from figure 4 is that at the lowest work functions, the probability for finding the atom in the Li(2p) state close to the surface is very small due to multi-state interactions.

Modeling - final Li(2p) occupancies versus $\Delta\Phi$:

We must now consider how the occupancies in the different atomic states evolve as the particle scatters from the surface, and the energies and widths of the atomic states change.

Information about the multi-state interactions that give rise to the peak in the Li(2p) yield with decreasing work function can be obtained from calculations like those shown in figure 5. The different curves in figure 5 show the probability of finding the atom in the Li(2p) state after it has scattered from the surface. Each curve corresponds to a calculation in which different states have been included. For example, the solid curve is with all states included, as discussed above. The dash-double-dotted (- . . - .) curve was done with the negative ion state excluded from the calculation. Note that removal of the negative ion state changes the Li(2p) yield significantly. In particular, with the negative ion state excluded, the Li(2p) yield is not zero at the lowest work functions. This is another manifestation of the competition between the Li(2p) and negative ion states at the lowest work functions.

The other two curves in figure 5 are Li(2p) yields calculated with *only* the Li(2s) and Li(2p) states included in the calculation. For the dash-dotted (- . - .) curve, the width of the Li(2p) level is greater than that of the Li(2s) at separations of a few to several angstroms from the surface, as shown in figure 3. Note that there is a peak in the Li(2p) yield at intermediate work functions. For the double-dashed dotted curve (- - . - -), we have set the width of the Li(2p) level equal to that of the Li(2s). For this latter calculation there is no peak in the Li(2p) yield, but rather a monotonic increase with decreasing work function. Thus we can also conclude that the relative widths of the alkali resonances, and how they vary with separation from the surface, are important in determining the final

electronic state occupancies in a scattering experiment.

To summarize, we conclude that multi-state "competition", for example between the negative ion and 2p state, is important in determining final state distributions. In addition, the z -dependence of the widths of the different states are important in describing the dynamics. The dynamics of the multi-state transfer are discussed in more detail elsewhere [8-12].

Other experimental and modeling trends:

Figure 2 shows Li(2p) yields for scattering with incident energies of 400 and 100 eV. The Li(2p) yield decreases with decreasing incident energy. The Li(2p) is an excited state which survives nonadiabatically; the lower the velocity, and the more adiabatic the system becomes, the smaller will be the Li(2p) yield. The model reproduces this trend. In addition, the peak in the Li(2p) yield occurs at a different work function shift $\Delta\Phi$ for the 400 and 100 eV scattering. This is also qualitatively reproduced by the model and can be understood by considering how the distance at which charge transfer occurs depends on the particle velocity and the resonance widths [11,12].

We have also made preliminary measurements for excited state formation in Na scattering. Figure 6 shows the relative yield of Na(3p) (excited state neutrals) versus the work function shift $\Delta\Phi$ for the scattering of 400eV Na⁺ from Cs-covered Cu(001). A rise in the yield of Na(3p) with decreasing work function is observed. The calculated Na(3p) yield using Marston's multi-state calculation is also shown as the solid line in figure 6. As expected from the discussion above, since the Na(3p) level is higher in energy than the Li(2p) level (by about 0.8 eV) the peak in the Na(3p) yield is shifted to lower work functions (larger $\Delta\Phi$). Note also that the shape of the measured Na(3p) yield is different than that for Li(2p) (compare figures 2 and 6), and different from that predicted by the model. We are in the process of making more careful measurements and calculations for the Na system.

Finally, recent progress has been made on upgrading the model. Marston and his collaborator, Alexey Onufriev, have expanded the number of states of the atom-metal system that can be included in the calculation. This upgrade has improved the accuracy of the calculation, and will enable us to include Auger neutralization processes (as well as the resonant processes already included) in the calculation. This is a particularly exciting development since only one other calculation we are aware of allows a simultaneous many body treatment of resonant and Auger processes [28].

Particle trapping and thin film growth modification at hyperthermal energies

As stated in section I of this report, we have recently begun a series of experiments to investigate the role of energetic particles in thin film growth. We have chosen 10 to 100 eV Na⁺ on Cu(100) as a model system, where we have extensive experience from both scattering experiments and computer simulations of the ion-surface collision process.

In order to assess the role of energetic particles in film growth, we need to understand *trapping and embedding* mechanisms in ion-surface interactions. A particle which loses so much energy that it cannot escape the substrate is considered *trapped* if it comes to rest within or above the outermost layer of surface atoms. It is *embedded* if it comes to rest

below the surface. For monoenergetic ions incident on a single crystal surface at a fixed incidence angle, we might expect the following behavior with incident energy. At very low energies, the surface corrugation is low, and forward scattering (i.e. smaller scattering angles) dominates. The incident particle transfers energy during its collision with the surface, and may become trapped in the attractive (in the case of alkalis on metals, image-like) surface potential. Surface penetration is not possible at these low energies, so the embedding probability is near zero. As the incident energy is raised, the particle scatters from the surface with enough kinetic energy to escape the surface potential, so the trapping probability begins to drop. As the incident energy is raised further, two things happen. The surface corrugation increases, allowing more violent (i.e. larger scattering angle) collisions between the incident particle and surface atoms, and thus correspondingly larger energy transfers. Also, penetration of the outermost layer of atoms becomes possible. Thus both the trapping and embedding probabilities increase. At the highest energies, most atoms penetrate, so the trapping again drops while embedding becomes more and more likely. We therefore expect the trapping probability to be large at the lowest energies, decrease with increasing energy, then possibly to increase again at some intermediate energy, before dropping off at the highest energies. The embedding should be zero at very low energies and increase essentially monotonically with energy.

Figure 7 shows calculated trapping and embedding probabilities for 10-200 eV Na^+ incident on Cu(001) along the $\langle 100 \rangle$ azimuth at a polar angle of 45° . The probabilities were calculated with SAFARI simulations [29] using an ion-surface potential determined from scattering experiments [30]. The simple ideas discussed above are borne out by the simulations. Note in particular that around 25 eV, the trapping probability becomes zero, and there is not yet appreciable embedding. As the energy is increased above 25 eV, more violent surface collisions become possible and the trapping probability begins to increase. Embedding does not appear until the energy has increased above approximately 50 eV. By 200 eV, the trapping probability has dropped nearly to zero, and only embedding remains as a mechanism for particle incorporation at the substrate.

We have made preliminary measurements of the *trapping* probability for these system using the technique of *resonant ion neutralization*. Sodium ions trapped on the copper surface have an appreciable dipole moment, which decreases the surface work function. This decrease is essentially linear for low coverages. Since the ion survival probability of *scattered* sodium drops dramatically as the surface work function decreases, monitoring the ion yield from the surface provides a sensitive measure of the coverage of trapped alkalis. This technique allows one to monitor the surface coverage in real time, as the same ion beam is being used for both deposition and measurement. We expect this technique to be mainly sensitive to *trapped* rather than embedded alkalis, since the more deeply embedded particles are screened and thus should have relatively small dipole moments. They should therefore contribute much less to the work function shift.

Figure 8 shows our measured trapping probabilities vs. the calculated trapping probabilities from figure 7. The trend with incident energy seems to be consistent with our calculations; note especially that the probability does seem to approach zero around 30 eV. However, we measure substantially less trapping than predicted. We are currently examining our ion-surface potential to see what changes might bring the calculated and measured

values into closer agreement. These changes must, of course, not change the very good agreement we have obtained between calculated and measured *scattering* distributions for this particular system.

In future experiments, we will measure the trapping and embedding as a function of the incident geometry and species. Simulations indicate that the probabilities are very sensitive to both. Additional experimental techniques will be used to monitor the surface coverages, such as Auger, thermal desorption, and work function measurements. These studies will be extended to other beams and surfaces, and STM will be used for *in-situ* studies of the ion-irradiated surfaces and deposited overlayers.

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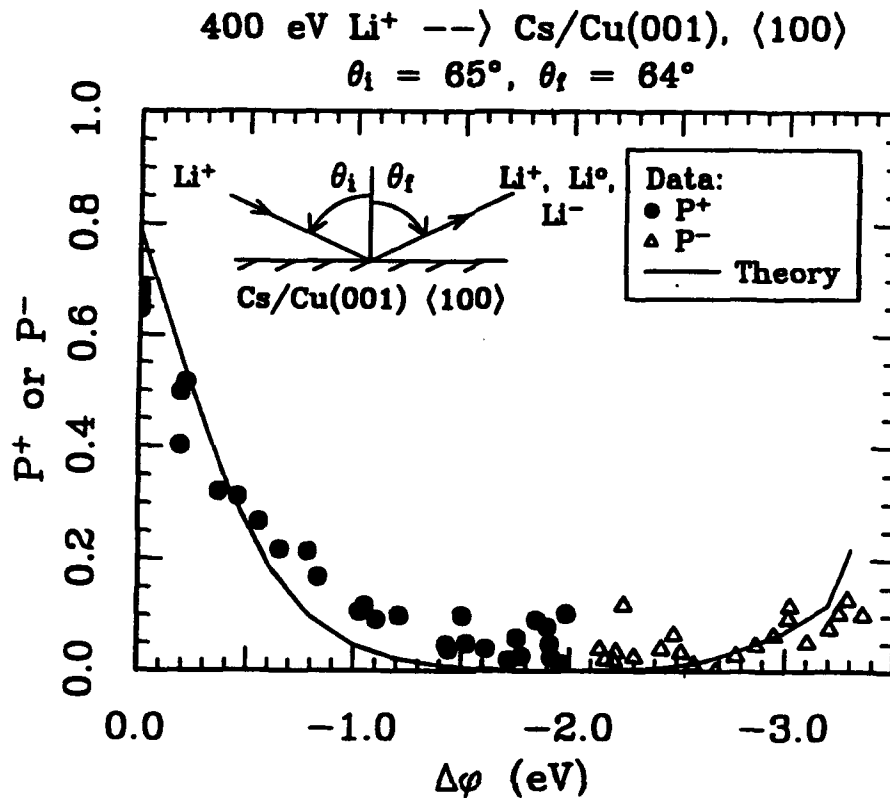


Figure 1: Measured and calculated values of the positive and negative charge state fractions for scattered Li versus the work function shift $\Delta\Phi$ induced by cesium adsorbates. Li^+ ions with an incident energy of 400eV impinge on a Cu(001) surface along the $\langle 100 \rangle$ azimuth with an incident angle of $\theta_i = 65^\circ$ measured with respect to the surface normal. Particles scattered into $\theta_f = 64^\circ$ are detected. $\Delta\Phi=0.0$ corresponds to the clean surface with $\Phi=4.59\text{eV}$. The solid circles indicate the measured positive ion fraction, P^+ , and the open triangles the negative ion fraction P^- . The calculated charge state fractions (solid line) were obtained using Marston's multi-state charge transfer model with alkali state energies and lifetimes from Nordlander and Tully.

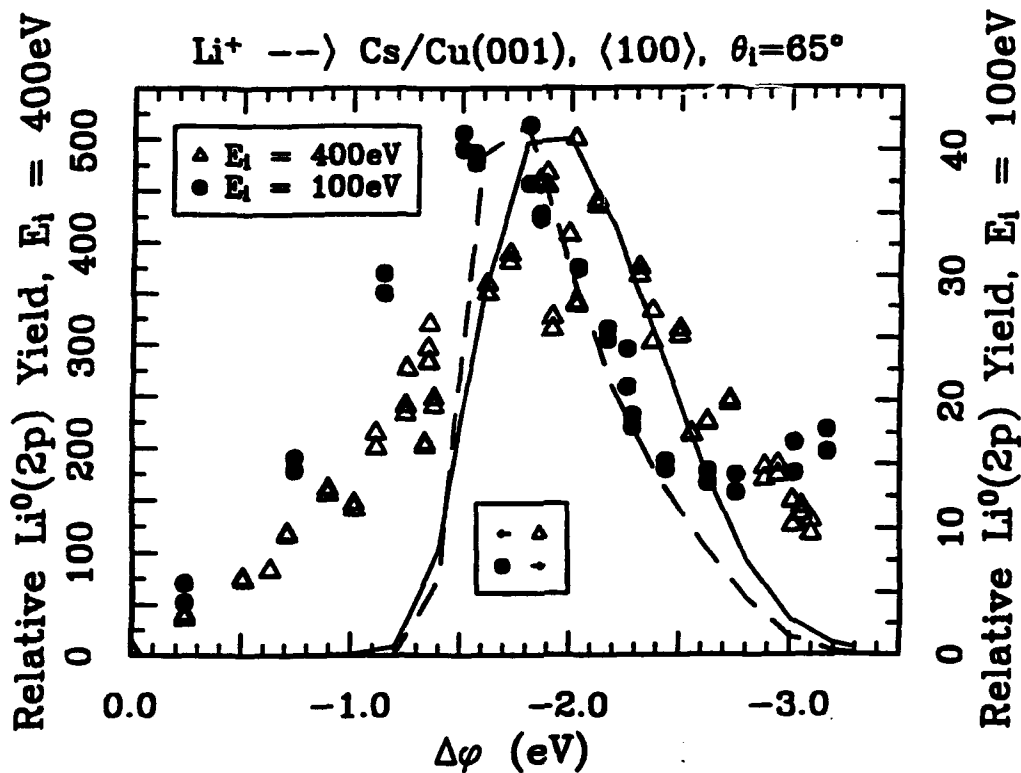


Figure 2: Measured and calculated values of the relative yield of excited neutral atoms in the Li(2p) state versus the work function shift $\Delta\Phi$ induced by cesium adsorbates. Li^+ ions with incident energies of 400 eV and 100 eV impinge on a Cu(001) surface along the $\langle 100 \rangle$ azimuth with an incident angle of $\theta_i = 65^\circ$ measured with respect to the surface normal. Photons corresponding to the Li(2p) \rightarrow Li(2s) transition ($\lambda = 673\text{nm}$) are detected. The two measured distributions for 400 eV (open triangles) and 100 eV (solid circles) have been normalized to one another; the yield at 100 eV is approximately an order of magnitude smaller than that at 400 eV. The calculated values were obtained using Marston's multi-state charge transfer model with alkali state energies and lifetimes from Nordlander and Tully. The calculated yields for 400 and 100 eV are given by the solid line and dashed line, respectively; the calculated ratio of the yield at 100 eV to that at 400 eV is similar to the measured ratio. The calculations also qualitatively reproduce the shift of the peak in $\Delta\Phi$ with decreasing beam energy.

The work function dependence of the Li(2p) yield can be understood as a multi-state effect in the charge transfer dynamics (see text).

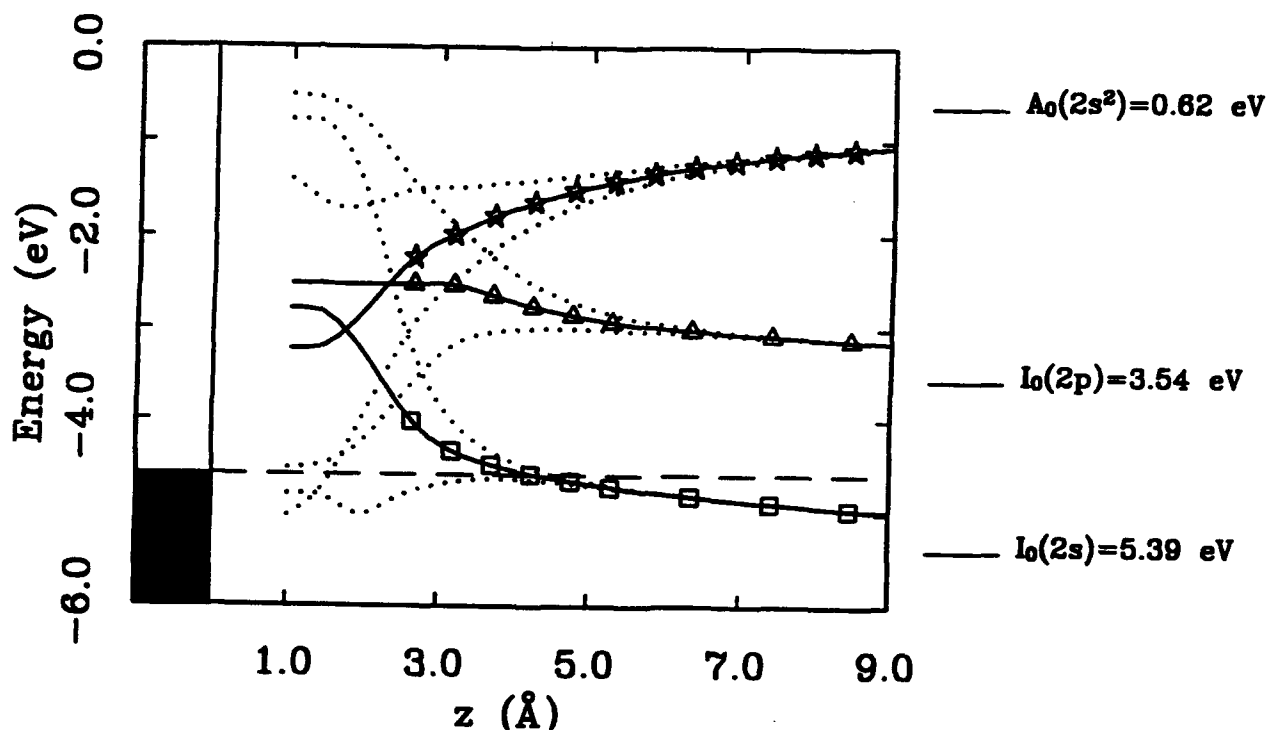


Figure 3: Calculated energies and level widths for Li near a Cu(001) surface. The open symbols show calculated values, obtained from Nordlander and Tully (NT), for the energies of the Li(2s) ground state ionisation level (squares), the Li(2p) excited state ionisation level (triangles), and the Li(2s²) affinity level (stars) at different distances from the surface. $z = 0$ corresponds to the jellium edge. The solid lines are spline fits to the NT calculations, which are chosen to saturate near the surface. The dotted curves show the widths of these levels as a function of z , also taken from NT calculations. The widths vary exponentially with separation from the surface, and saturate near the surface.

The shaded region on the left of the diagram ($z < 0$) shows the filled conduction band of clean Cu(001). The top of the shaded region represents the Fermi energy, which lies an energy of $\Phi = 4.59$ eV (the work function of clean Cu(001)) below the vacuum energy of 0 eV. When alkali adsorbates are deposited on the Cu(001) surface, the work function decreases (i.e., the Fermi energy shifts up on this diagram). The minimum work function obtained in the experiment was approximately 1.4 eV (i.e., a work function shift of approximately 3.2 eV).

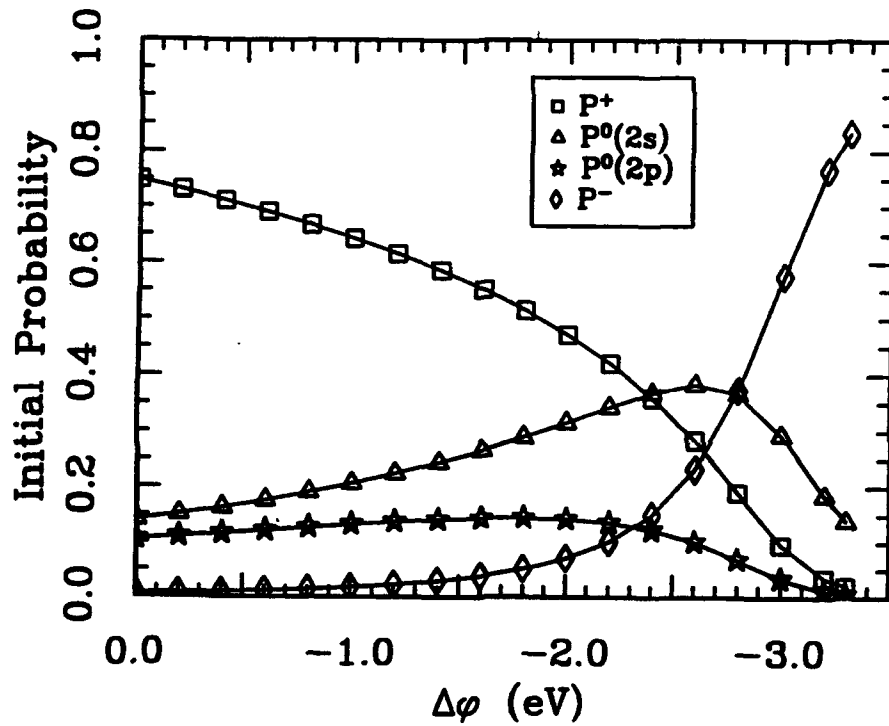


Figure 4: Calculated probabilities for finding the Li atom in the positive ion (P^+), negative ion (P^-), 2s ($P^-(2s)$), or 2p ($P^-(2p)$) states for an atom-surface separation of 1\AA . These probabilities correspond to the electronic adiabatic ground state for the Li close to the surface. The calculations were done using Marston's multi-state model (see text).

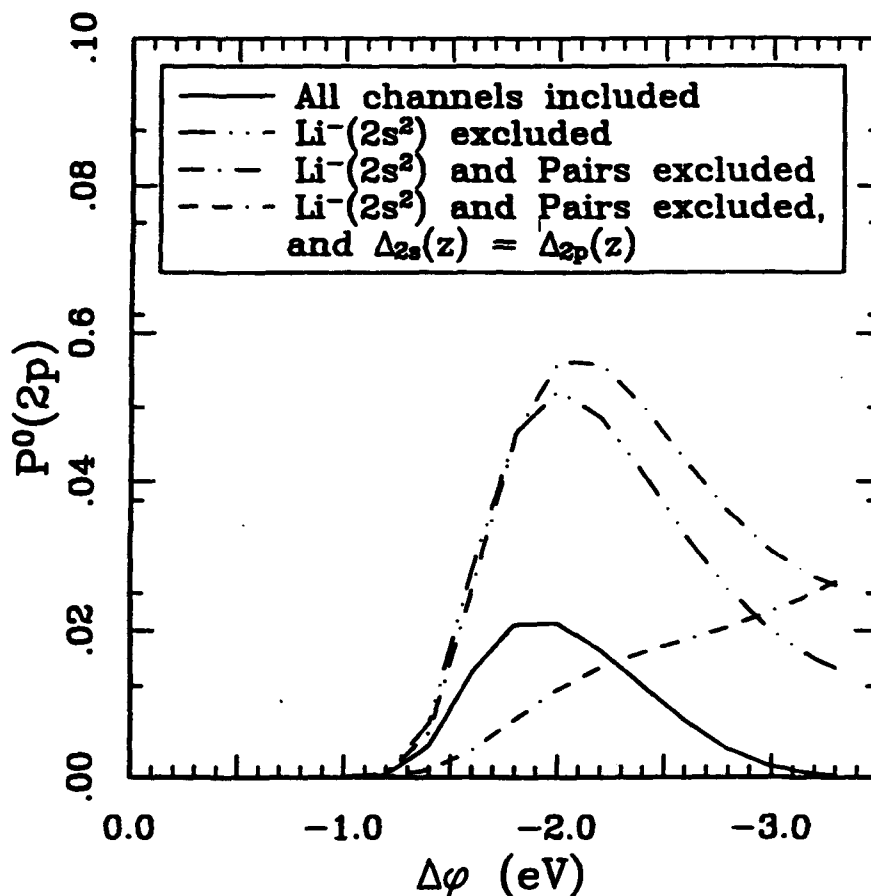


Figure 5: Calculated probabilities for finding the Li atom in the 2p state after it has scattered from the surface. The velocity in the calculation corresponds to the scattered velocity for 400 eV incident Li^+ . The calculations were done using Marston's multi-state charge transfer code. The different curves correspond to calculations in which different states have been included. These curves illustrate the sensitivity of the multi-state charge transfer dynamics to which combinations of state are considered, and to the relative widths of the different states and how they vary with distance from the surface (see text).

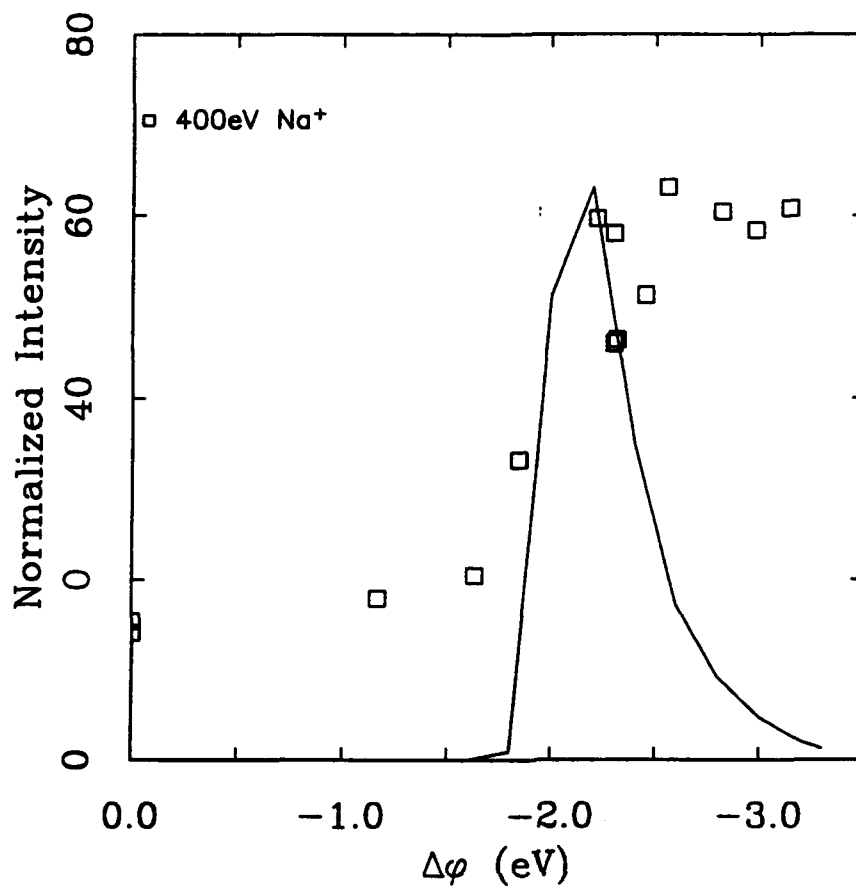


Figure 6: Measured and calculated values of the relative yield of excited neutral atoms in the Na(3p) state versus the work function shift $\Delta\Phi$ induced by cesium adsorbates. Na⁺ ions with incident energies of 400eV impinge on a Cu(001) surface along the $\langle 100 \rangle$ azimuth with an incident angle of $\theta_i = 65^\circ$ measured with respect to the surface normal. Photons corresponding to the Na(3p) \rightarrow Na(3s) transition ($\lambda = 589\text{nm}$) are detected. The calculated values were obtained using Marston's multi-state charge transfer model with alkali state energies and lifetimes from Nordlander and Tully. The calculated curve is normalized to the data.

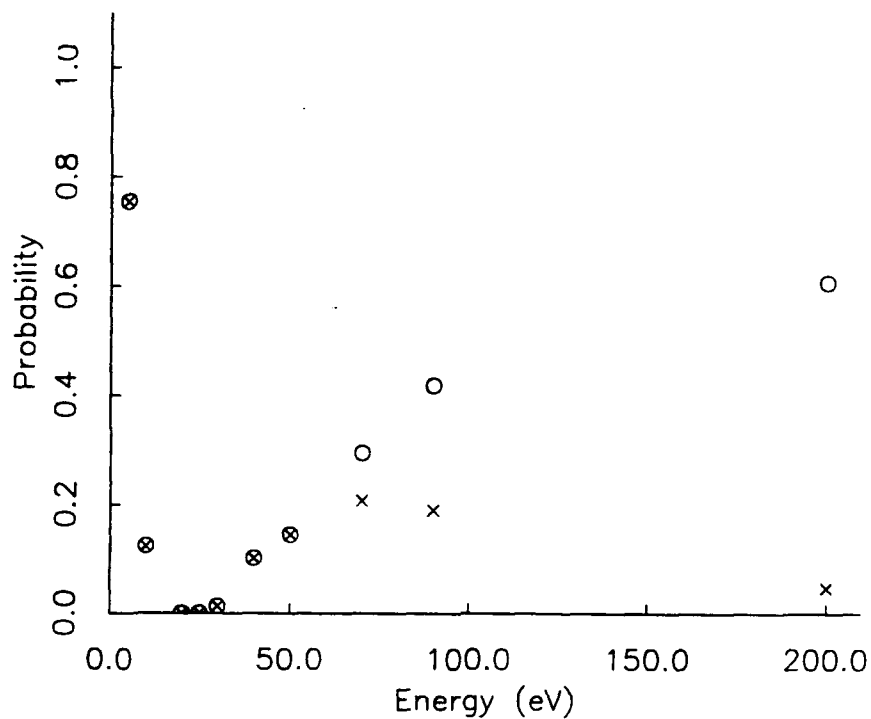


Figure 7: Calculated trapping and embedding probabilities for Na^+ incident on the (001) azimuth of Cu(100) at a polar angle of 45° , as a function of energy. (x) – trapping probability. (o) – trapping plus embedding probability. The embedding probability is simply the difference between the two curves. The calculations were made using the SAFARI simulation of ion-surface scattering (see text).

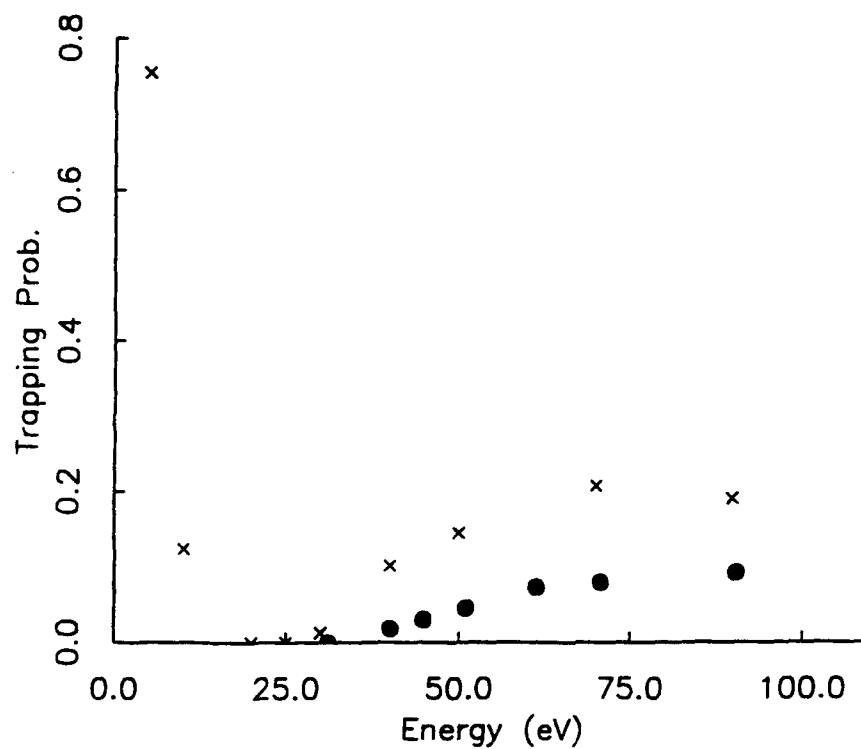


Figure 8: Comparison between calculated (x) and measured (•) trapping probabilities for Na⁺ incident on the (001) azimuth of Cu(100) at a polar angle of 45°, as a function of energy (see text).

VI. RESEARCH PARTICIPANTS

Participants in the charge exchange research program include B.H. Cooper (partial summer salary from AFOSR-91-0137) and graduate students G.A. Kimmel, D.R. Peale, S.T. Tsao, and C. Wengel and postdoctoral fellow D. Goodstein (supported by AFOSR-91-0137). Graduate students E. Behringer (supported by MSC-NSF-DMR-8516616) and C. Keller (supported by a Hertz Fellowship), and postdoctoral fellow D. Andersson (supported by the Sweden-America Foundation and NSF) are also working on charge transfer. Also working on the apparatus and involved in related research programs are graduate students J. McLean (supported by AASERT) and E. Dahl (supported by an AT&T Fellowship). Brad Marston from Brown University is collaborating with us on theoretical modeling of charge transfer processes.

VII. PUBLICATIONS

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- 22) "Probing Surface Lattice Dynamics with Hyperthermal Ion Scattering," D.M. Goodstein, C.A. DiRubio, B.H. Cooper, and K. Burke, *Surface Reviews and Letters*, in press.
- 23) "Energy Transfer, Trapping, and the Attractive Well in Hyperthermal Na^+ Scattering from Cu(001) Part I, Dynamics," in preparation.
- 24) "Energy Transfer, Trapping, and the Attractive Well in Hyperthermal Na^+ Scattering from Cu(001): Part II, The Interactions Potential," in preparation.

- 25) "Quantitative Detection of Low Energy Positive and Negative Ions with a Channel Electron Multiplier," C.A. Keller and B.H. Cooper, in preparation.
- 26) "Charge Transfer in Low Energy Scattering of O^+ from Cu(001)," C.A. Keller and B.H. Cooper, in preparation.
- 27) "Surface Dynamics Probed with Hyperthermal Energy Ion Scattering," C.A. DiRubio, D.M. Goodstein, and B.H. Cooper, in preparation.
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- 29) "Multi-Channel Charge Transfer in Li^+ Scattering with Alkali-Covered Cu(001) II. The Dynamics of Excited State Formation," in preparation.
- 30) "Energy and Angular distributions of 100 and 400 eV Li Scattering from Cu(001)," E.R. Behringer, J.G. McLean, and B.H. Cooper.
- 31) "Mass Flow from Nonequilibrium Nano-Structures on the Au(111) Surface Observed by Scanning Tunneling Microscopy," D.R. Peale, J.G. McLean, R. Phillips, E. Chason, and B.H. Cooper, in preparation.
- 32) "Trajectory-Dependent Charge Transfer in Hyperthermal Energy Scattering of Na^+ from Cu(001)," C.A. Keller, C.A. DiRubio, and B.H. Cooper, in preparation.

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- 33) "Scattering and Charge Transfer Dynamics in Low and Hyperthermal Energy Alkali Ion-Surface Collisions," B.H. Cooper and E.R. Behringer, p. 264-312, in *Low Energy Ion-Surface Interactions, Advances in Ion Chemistry and Physics*, J. Wayne Rabalais (ed.), John Wiley & Sons, Ltd: Sussex, 1994.

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"Trajectory and Impact Parameter Analysis of Hyperthermal Ion Scattering," Randall L. McEachern, Cornell Physics Ph.D. Thesis (1990).

"Energy and Charge Transfer in Hyperthermal Ion-Surface Scattering," David M. Goodstein, Cornell University Ph.D. Thesis (1990).

"Diffusion and Mass Flow Dynamics on the Gold(111) Surface Observed by Scanning Tunneling Microscopy," David Reese Peale, Cornell Physics Ph.D. Thesis (1992).

"The Dynamics of Resonant Charge Exchange in Low Energy Ion-Surface Interactions," Gregory Allen Kimmel, Cornell Physics Ph.D. Thesis (1992).

"The Dynamics of Energy Transfer in Hyperthermal Energy Ion Scattering from Metal Surfaces," Christopher Auguste DiRubio, Cornell Physics Ph.D. Thesis (1993).

"The Dynamics of Resonant Charge Transfer in Hyperthermal Energy Ion-Surface Collisions," Ernest Robert Behringer, Cornell Physics Ph.D. Thesis (1994).

VIII. PRESENTATIONS

- 1) Computer Simulations of Hyperthermal Ion Scattering: Measuring Short-Range Surface Order in Crystals,
B.H. Cooper and D.M. Goodstein, presented at the Sixth International Workshop on Inelastic Ion Surface Collisions, Argonne National Laboratory, August 1986. (poster presentation)
- 2) Hyperthermal Ion-Surface Scattering Simulation: Alternatives to Monte Carlo,
D.M. Goodstein, S.A. Langer, and B.H. Cooper, presented at the New York Meeting of the American Physical Society, March 1987. (poster presentation)
- 3) A Versatile Apparatus for Low Energy and Hyperthermal Ion Scattering,
R.L. McEachern and B.H. Cooper, presented at the New York meeting of the American Physical Society, March 1987. (oral presentation)
- 4) An Ion Scattering System for the Energy Range 10 eV to 10 keV,
D.L. Adler and B.H. Cooper, presented at the New York meeting of the American Physical Society, March 1987. (oral presentation)
- 5) Ion-Surface Scattering at Low and Hyperthermal Energies: Scattering Dynamics and Charge Exchange in Relation to Surface Chemistry,
B.H. Cooper, invited talk at the American Chemical Society Meeting, New Orleans, September 1987.
- 6) Ion Surface Scattering at Hyperthermal Energies: Scattering Dynamics and Charge Exchange,
B.H. Cooper, talk at the AFOSR Surface Chemistry Contractor's Conference, Colorado Springs, September 1987.
- 7) Interactions of Hyperthermal Ion Beams with Metal Surfaces,
D.M. Goodstein, R.L. McEachern, and B.H. Cooper, presented at the 34th National Symposium of the American Vacuum Society, Anaheim, California, November 1987. (poster presentation)
- 8) Design and Performance of Ion Optics for Hyperthermal (10-100 eV) and keV Ion Scattering,
D.L. Adler, B.H. Cooper, and D.R. Peale, presented at the 34th National Symposium of the American Vacuum Society, Anaheim, California, November 1987. (poster presentation)
- 9) Scattering Dynamics of Low Energy Alkali and Noble Gas Ions Incident on Cu(110),
R.L. McEachern, D.L. Adler, D.M. Goodstein, G.A. Kimmel, and B.H. Cooper, presented at the New Orleans meeting of the American Physical Society, March 1988. (oral presentation)
- 10) Low Energy Ion Scattering Studies of Surfaces Disordered by Ion Bombardment,
G.A. Kimmel, D.L. Adler, D.M. Goodstein, R.L. McEachern, and B.H. Cooper, presented at the New Orleans meeting of the American Physical Society, March

1988. (oral presentation)
- 11) Structural Study of the O/Cu(110) System Using Hyperthermal and Low Energy Noble Gas and Alkali Ion Scattering,
D.L. Adler, R.L. McEachern, D.M. Goodstein, G.A. Kimmel, and B.H. Cooper, presented at the New Orleans meeting of the American Physical Society, March 1988. (oral presentation)
 - 12) Hyperthermal Alkali Ion Scattering from Cu(110),
D.M. Goodstein, D.L. Adler, R.L. McEachern, and B.H. Cooper, presented at the New Orleans meeting of the American Physical Society, March 1988. (oral presentation)
 - 13) Low and Hyperthermal Energy Ion-Surface Scattering: Trajectory Analysis, Multiple Scattering, and Charge Exchange,
B.H. Cooper, invited talk at Rutgers University, Piscataway, NJ, April 1988.
 - 14) Scattering of 50 eV to 4 keV Alkali Ion Beams from Cu(110) Surfaces: Trajectory Analysis and Charge Exchange.
B.H. Cooper, invited talk at Xerox Corporation, Webster, NY, June 1988.
 - 15) Ion-Surface Scattering at Hyperthermal and keV Energies: Interaction Potentials, Trajectory Analysis, and Charge Exchange,
B.H. Cooper, talk at the 48th Annual Conference on Physical Electronics, Brookhaven Labs, June 1988.
 - 16) Low Energy Ion Scattering as a Probe of Resonant Charge Exchange on Cu(110),
G.A. Kimmel, R.L. McEachern, D.L. Adler, D.M. Goodstein, B.H. Cooper, presented at the 35th National Symposium of the American Vacuum Society, Atlanta, Georgia, October 1988. (oral presentation)
 - 17) Hyperthermal Na⁺ and K⁺ Scattering as a Probe of Resonant Charge Exchange on Cu(110),
D.M. Goodstein, R.L. McEachern, B.H. Cooper, presented at the 35th National Symposium of the American Vacuum Society, Atlanta, Georgia, October 1988. (poster presentation)
 - 18) Third Annual AFOSR Workshop on "Surface Reactions in a Space Environment",
B.H. Cooper, invited talk, Vanderbilt University Center for Atomic and Molecular Physics at Surfaces, Nashville, TN, October 1988.
 - 19) Alkali Ion-Surface Scattering at Hyperthermal Energies,
B.H. Cooper, AFOSR Molecular Dynamics Contractors Conference, Newport Beach, CA, October 1988. (poster presentation)
 - 20) Low Energy Ion Beam Scattering as a Probe of Ion-Surface Interactions,
B.H. Cooper, invited talk, Michigan State University, Condensed Matter Physics Seminar, February 1989.

- 21) Ion-Surface Interactions at Hyperthermal Energies: Scattering and Charge Transfer Mechanisms,
B.H. Cooper, invited talk, presented at the St. Louis Meeting of the American Physical Society, March 1989.
- 22) Elastic and Inelastic Processes in Hyperthermal Ion-Surface Interactions,
D.M. Goodstein, G.A. Kimmel, B.H. Cooper, B. Kasemo, presented at the St. Louis Meeting of the American Physical Society, March 1989. (oral presentation)
- 23) 100 to 400 eV Na^+ Scattering from Cu(110),
D.L. Adler, D.M. Goodstein, and B.H. Cooper, presented at the St. Louis Meeting of the American Physical Society, March 1989. (oral presentation)
- 24) Low-Energy Ion Beam Scattering as a Probe of Ion-Surface Interactions,
B.H. Cooper, invited talk, Molecular Beams Group of the Royal Society of Chemistry, Meeting on "Ions, Clusters, and Surfaces," Liverpool, England, April 1989.
- 25) Low and Hyperthermal Energy Ion Scattering Studies of Charge Transfer at Clean and Adsorbate-Covered Metal Surfaces,
B.H. Cooper, invited talk, Workshop on "Dynamics of Surface Reactions," Copenhagen, Denmark, May 1989.
- 26) A Vibration-Insensitive Thermally-Compensated Scanning Tunneling Microscopy for UHV Surface Studies,
D.R. Peale and B.H. Cooper, presented at the Scanning Tunneling Microscope Spring Workshop, University of Pennsylvania, Philadelphia, PA, May 1989. (poster presentation)
- 27) Hyperthermal Ion Scattering: Trajectory Analysis
R.L. McEachern, Ph.D. job talk presented at AT&T Bell Laboratories, Murray Hill, NJ, April 1989; IBM Yorktown Heights, NY, April 1989; IBM Almaden, CA, May 1989; Sandia National Laboratories, Albuquerque, NM, May 1989.
- 28) A Scanning Tunneling Microscope for UHV Atom-Surface Interaction Studies,
D.R. Peale and B.H. Cooper, presented at the 4th International Conference on Scanning Tunneling Microscopy, Oarai, Japan, July 1989. (poster presentation)
- 29) Hyperthermal Energy Ion Scattering as a probe of Charge Transfer at Surfaces,
B.H. Cooper, invited talk, Gordon Conference on "Dynamics of Gas-Surface Interactions," Proctor Academy, Andover, NH, August 1989.
- 30) The Influence of Adsorbate-Induced Local Electronic Structure on Charge Exchange Processes at Surfaces,
G.A. Kimmel, D.M. Goodstein, B. Kasemo, and B.H. Cooper, presented at the Gordon Conference on "Dynamics of Gas-Surface Interactions," Proctor Academy, Andover, NH, August 1989. (poster presentation)
- 31) 10-100 eV Ion-Surface Interactions: Measurements and Classical Trajectory Simulations,

B.H. Cooper, invited talk, AFOSR Fourth Annual Workshop on Surface Reactions in the Space Environment, Northwestern University, September 1989.

- 32) The Influence of Local Electronic Structure on the Neutralization of Alkali Ions Scattered from Adsorbate-Covered Cu(001),
G.A. Kimmel, D.M. Goodstein, B. Kasemo, and B.H. Cooper, presented at the 36th National Symposium of the American Vacuum Society, Boston, MA, October 1989. (poster presentation)
- 33) Hyperthermal Energy Ion Scattering from the (2×1) Oxygen Reconstructed Surface of Cu(110),
D.L. Adler, D.M. Goodstein, and B.H. Cooper, presented at the 36th National Symposium of the American Vacuum Society, Boston, MA, October 1989. (oral presentation)
- 34) A Scanning Tunneling Microscope for UHV Surface Studies,
D.R. Peale and B.H. Cooper, presented at the Cornell National Nanofabrication Facility, 11th Annual Industrial Affiliates Meeting, October 1989. (oral presentation)
- 35) Local Adsorbate-Induced Effects on Non-Adiabatic Charge Transfer to Hyperthermal Energy Ions,
B.H. Cooper, talk at the AFOSR Molecular Dynamics Contractors Conference, Captiva Island, Florida, October 1989.
- 36) Energy, Momentum, and Charge Transfer in Hyperthermal Ion-Surface Interactions,
D.M. Goodstein, Ph.D. job talk presented at University of Washington, Dept. of Chemistry, June 1989; AT&T Bell Laboratories, Holmdel, NJ, September 1989; IBM Yorktown Heights, NY, October 1989.
- 37) Dynamical Charge Transfer in Ion-Surface Interactions,
B.H. Cooper, invited talk, Physical Chemistry Seminar, Penn State University, November 1989.
- 38) Energy and Charge Transfer Mechanisms in Ion-Surface Collisions,
B.H. Cooper, Bell Laboratories, General Physics Colloquium, Murray Hill, NJ, April 1990.
- 39) Energy and Charge Transfer Mechanisms in Ion-Surface Collisions,
B.H. Cooper, Physics Department Colloquium, University of Virginia, Charlottesville, VA, April 1990.
- 40) Energy and Charge Transfer Mechanisms in Ion-Surface Collisions,
B.H. Cooper, Chalmers University of Technology, Solid State Physics Seminar, Gothenburg Sweden, June 1990.
- 41) Energy and Charge Transfer Mechanisms in Ion-Surface Collisions,
B.H. Cooper, Liverpool Surface Science Research Centre, Seminar, University of Liverpool, June 1990.

- 42) Hyperthermal Energy Ion Scattering as a Probe of Charge Transfer at Surfaces,
B.H. Cooper, invited talk at the Particle-Solid Gordon Conference, Plymouth,
New Hampshire, July 1990.
- 43) Energy and Charge Transfer Mechanisms in Ion-Surface Collisions,
B.H. Cooper, invited talk at the Gas-Surface Dynamics Symposium of the Amer-
ican Chemical Society, Washington, DC, August 1990.
- 44) Energy and Charge Transfer Mechanisms in Ion-Surface Collisions at Hyperthermal
Energies,
B.H. Cooper, invited talk at the Workshop on Surface Reactions in the Space
Environment, Evanston, Illinois, September 1990.
- 45) Ion-Surface Interactions and Scattering Dynamics,
B.H. Cooper, General Physics Colloquium, Cornell University, December 1990.
- 46) Ion-Surface Interactions and Scattering Dynamics,
B.H. Cooper, Colloquium, Laboratory for Research on the Structure of Matter
and Department of Materials Science and Engineering, University of Pennsylva-
nia, December 1990.
- 47) Ion-Surface Interactions and Scattering Dynamics,
B.H. Cooper, invited talk at the Center for Chemical Physics - Surface Science
Division, National Institute of Standards and Technology, Gaithersburg, MD,
December 1990.
- 48) Hyperthermal Na^+ Scattering Distributions from $\text{Cu}(001)$: The Role of the Attractive
Interaction,
C.A. DiRubio and B.H. Cooper, contributed talk at the American Physical Soci-
ety Meeting, Cincinnati, OH, March 1991.
- 49) Cross Sections for Non-Adiabatic Resonant Charge Transfer for Li, Na, and K on
 $\text{Cu}(001)$,
G.A. Kimmel, J.B. Marston, and B.H. Cooper, contributed talk at the American
Physical Society Meeting, Cincinnati, OH, March 1991.
- 50) Non-Adiabatic Charge Transfer in O^+ and O_2^+ Scattering from Clean and Adsorbate-
Covered $\text{Cu}(001)$,
C.A. Keller and B.H. Cooper, contributed talk at the American Physical Society
Meeting, Cincinnati, OH, March 1991.
- 51) A Many-Body Theory of Charge Transfer in Hyperthermal Atomic Scattering,
J. Brad Marston, Cliff Richardson, Ernie Behringer, Greg A. Kimmel, and Bar-
bara H. Cooper, contributed talk at the American Physical Society Meeting,
Cincinnati, OH, March 1991.
- 52) Formation of Excited States in Li^+ -Surface Collisions Via Resonant Charge Transfer,
E.R. Behringer, D. Andersson, and B.H. Cooper, contributed talk at the Ameri-
can Physical Society Meeting, Cincinnati, OH, March 1991.

- 53) Surface Self-Diffusion on Au(111) Observed by Scanning Tunneling Microscopy,
D.R. Peale and B.H. Cooper, contributed talk at the American Physical Society Meeting, Cincinnati, OH, March 1991.
- 54) Non-Adiabatic Resonant Neutralization of Alkali Ions Scattered from Cu(100),
G.A. Kimmel, J.B. Marston, and B.H. Cooper, invited talk at the European Science Foundation Workshop on Charge Transfer Phenomena at Surfaces (presented by G. Kimmel for B. Cooper), Noordwijkerhout, The Netherlands, May 1991.
- 55) Low Energy Ion-Surface Interactions,
C.A. DiRubio, G.A. Kimmel, J.B. Marston, and B.H. Cooper, invited talk at the 10th International Conference on Ion Beam Analysis (presented by C. DiRubio for B. Cooper), Eindhoven, The Netherlands, July 1991.
- 56) The Dynamics of Hyperthermal Alkali Ion-Surface Interactions,
B.H. Cooper, D. Andersson, E.R. Behringer, C.A. DiRubio, and G.A. Kimmel, invited talk at the 12th European Conference on Surface Science (presented by E. Behringer for B. Cooper), Stockholm-Uppsala, Sweden, September 1991.
- 57) Charge Transfer and Trapping Dynamics in Hyperthermal Ion-Surface Collisions,
B.H. Cooper, invited talk at the 6th Annual Workshop on Surface Reactions in the Space Environment, Evanston, Illinois, September 1991.
- 58) Multi-Channel Charge Transfer Reactions at Surfaces,
B.H. Cooper, D. Andersson, E.R. Behringer, G.A. Kimmel, C. Keller, and J.B. Marston, talk at the AFOSR Molecular Dynamics Contractors Conference, Irvine, California, October 1991.
- 59) Dynamics of Hyperthermal Ion-Surface Collisions,
March Meeting of the American Physical Society, Indianapolis, IN, March 1992, Maria-Goeppert Mayer Award Talk.
- 60) Women in Physics: The View from a Research University,
March Meeting of the American Physical Society, Indianapolis, IN, March 1992, CSWP sponsored panel discussion on Women Physicists: Observations of the Changing Mileu - Now and Then.
- 61) STM Observations of Adsorbate-Promoted Mass Flow on the Au(111) Surface,
D.R. Peale, J.G. Mclean, B.H. Cooper, contributed talk at the 1992 March Meeting of the American Physical Society, Indianapolis, IN, March 1992.
- 62) What Happens When Low Energy Ions Collide With Surfaces: From the Space Shuttle to Surface Processing,
Colgate University, Physics Department Seminar, April 1992.
- 63) What Happens When Low Energy Ions Collide with Surfaces: From the Space Shuttle to Surface Processing,
General Electric, Colloquium, Schenectady, NY, April 1992.

- 64) Ion-Surface Charge Transfer Dynamics,
American Physical Society, Annual Meeting of the Division of Atomic, Molecular,
and Optical Physics, Chicago, IL, May 1992.
- 65) Mass Flow and Stability of Nanoscale Features on Au(111): The Role of Adsorbates,
DOE Sponsored Workshop on Surface Diffusion and the Growth of Materials,
Santa Fe, NM, June 1992.
- 66) Charge Transfer in Ion-Surface Scattering,
Ninth International Workshop on Inelastic Ion Surface Collisions, Aussois, France,
September 1992.
- 67) Charge State-Resolved Scattering Measurements: Probing the Dynamics of Hyper-
thermal Energy Atom-Surface Interactions,
Seventh Annual Workshop on Surface Reactions in the Space Environment, Skokie,
IL, September 1992.
- 68) Positive to Negative Scattered Ion Ratios in Nonadiabatic O^+ Scattering from Cu(001),
C.A. Keller and B.H. Cooper, March Meeting of the American Physical Society,
Indianapolis, IN, March 1992.
- 69) The Influence of Charge Exchange and Surface Vibrations on Hyperthermal Alkali
Ion Scattering Distribution from Cu(001),
C.A. DiRubio, G.A. Kimmel, and B.H. Cooper, March Meeting of the American
Physical Society, Indianapolis, IN, March 1992.
- 70) The Dynamics of Low Energy Li^+ Scattered from Cu(001),
E.R. Behringer and B.H. Cooper, March Meeting of the American Physical So-
ciety, Indianapolis, IN, March 1992.
- 71) Adsorbate Dependence of the Formation of Excited States in Alkali Ion-Surface Col-
lision,
D.R. Andersson, E.R. Behringer, B.H. Cooper, and J.B. Marston, March Meeting
of the American Physical Society, Indianapolis, IN, March 1992.
- 72) Charge Transfer in Low Energy Collisions of Li^+ with Adsorbate-covered Cu(001),
E.R. Behringer, D.R. Andersson, B.H. Cooper, and J.B. Marston, 52nd Physical
Electronics Conference, Irvine, CA, June 1992.
- 73) Velocity Dependence of Final State Formation in Low Energy Li^+ -Surface Collisions,
D.R. Andersson, E.R. Behringer, B.H. Cooper, and J.B. Marston, 39th National
Symposium of the American Vacuum Society, November 1992, Chicago, IL.
- 74) Mass Flow and Stability of Nanoscale Features on Au(111),
Fall Meeting of the Materials Research Society, Boston, MA, December 1992.
- 75) What Happens when Hyperthermal Ions Collide with Surfaces,
Rice University, Physics Department Colloquium, Houston, TX, April 1993.
- 76) Multi-Channel Charge Transfer Dynamics in Atom-Surface Scattering,

Workshop on Vibronic Processes in Gas Phase and Surface Scattering, Pousada de Palmela, Portugal, May 1993.

- 77) Energy and Charge Transfer Dynamics in Hyperthermal Energy Ion-Surface Collisions,
Laboratoire des Collisions Atomiques et Moleculaires, Laboratory Seminar, Universite Paris-Sud, Orsay, France, May 1993.
- 78) Materials Science at a Surface,
Cornell Materials Science Center Summer Research Experience for Undergraduate Program, Ithaca, NY, June 1993.
- 79) Ion-Surface Collisions: Probing the Dynamics of Energy and Charge Transfer,
Caltech Physics Colloquium, October 1993.
- 80) Ion-Surface Interactions: Applications to Thin Film Growth,
B.H. Cooper, talk at the AFOSR Surface Chemistry Contractor's Conference, Irvine, CA, October 1993.
- 81) Scanning Tunneling Microscopy for Materials Analysis,
Cornell College of Human Ecology, Department of Textiles and Apparel Colloquium, April 1994.
- 82) Atom-Surface Interactions: Probing Dynamics with Ion Scattering,
Brown University Physics Department Colloquium, Providence, RI, April 1994.
- 83) Interactions of Slow Alkali Ions with Surfaces: Charge Transfer Dynamics,
Particle-Solid Interactions Gordon Conference, Plymouth NH, August 1994.
- 84) Interactions of Hyperthermal Alkali Ions with Surfaces: Charge Transfer Dynamics,
Seminar, Department of Applied Physics, Chalmers University of Technology, Gothenburg, Sweden, August 1994.
- 85) Charge Transfer Dynamics in Ion-Surface Scattering,
European Science Foundation Conference on Electronic Structure of Solids: Dynamics and excitations, Gausdal, Norway, August 1994.